51006	Species Name:	HCCNC-v6
1		Ethynyl-isocyanide,
Jan. 1995		$\nu_6$ vibrational state
M. L. Delitsky		
H. M. Pickett		
291	Q(300.0) =	3775.7021
983.83	Q(225.0) =	2832.7507
99	Q(150.0) =	1888.7322
-10.0	Q(75.00) =	944.7917
-100.0	Q(37.50) =	472.8781
0.0	Q(18.75) =	236.9363
424.0	Q(9.375) =	118.9708
2.93	A=	
	B=	4978.500
	C=	
	1 Jan. 1995 M. L. Delitsky H. M. Pickett 291 983.83 99 -10.0 -100.0 0.0 424.0	1 Jan. 1995 M. L. Delitsky H. M. Pickett 291 983.83 Q(225.0)= 99 Q(150.0)= -10.0 Q(75.00)= -100.0 Q(37.50)= 0.0 Q(18.75)= 424.0 Q(9.375)= 2.93 A= B=

The observed frequency measurements were taken from A. Guarnieri, R. Hinze, M. Krüger and H. Zerbe-Foese, 1992, J. Mol. Spect. **156**, 39. The  $\nu_6$  vibration is a low lying excited bending state at 424 cm<sup>-1</sup>. It should be noted that the  $\nu_6$  is an l doubled state.

The dipole moment was assumed to be the same as for the ground state. M. Krüger, H. Dreizler, D. Preugschat and D. Lentz, 1991, Angew. Chem. Int. Ed. Engl. **30**, 1644.